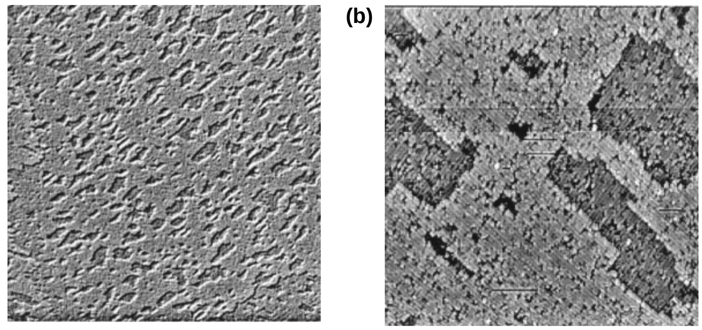
Atomistic Evaluation of Surface and Interface Processes

Atomic-level control of nanostructures and thin films

Development of new, high-performance materials in several critical technologies—microelectronics, multilayer systems, and composites, for example—requires precise, atomistic control over interfacial composition and structure. We have developed a facility for optimizing these new materials. At LLNL, a single ultra-high-vacuum system allows us to provide

- Facilities for preparing atomically clean surfaces with rapid sample introduction
- Ion sputtering and epitaxial deposition capabilities commonly used for interface modification and film growth
- Quantitative, low-energy electron diffraction and real-time, high-energy electron diffraction for structure determination through k-space analysis both during and after interface modification
- Atomic-resolution tunneling microscopy (STM) for real-space, surface-structure determination.

(a) (b)



4200 Å

700 Å detail

STM images of Si(100)-2 x 1 following 200-eV xenon sputtering at 436°C. (a) 4200-Å image after removal of one-third of monolayer; (b) 700-Å detail showing the newly exposed dimer rows.

APPLICATIONS

- *In-situ real-space (by STM) and k-space (by electron diffraction) structural evaluation*
- *Comprehensive diagnosis of surface processes*
- *Diagnosis of critical epitaxial processes that require an ultra-high-vacuum environment*

Diagnostic capabilities combined with rapid sample turnaround and a flexible deposition capability enables a more direct route to improved surface processing. We can, for example, investigate what happens to surface structural characteristics (such as defect densities) when we adjust processing parameters (such as deposition rates or substrate temperature).

Current experiments

We have characterized the effects of low-energy ion sputtering of silicon. Ion sputtering is commonly used by the semiconductor industry to clean silicon surfaces; however, the microscopic effects of low-energy (<200 eV) irradiation have only recently been investigated.

This technique offers promise for deliberate modification of silicon surfaces. When electron diffraction indicates a layer-by-layer mode of sputtering, STM images acquired after ion exposure (see the accompanying figure) reveal the sizes, shapes, and distribution of monolayer-deep surface depressions. The STM images in the figure display, on two different length scales, the atomic ordering on a Si(100) surface after removal of approximately one-third of the monolayer by 200-eV xenon sputtering at 436°C. The image displays the individual dimer rows in both the outermost atomic layer and the monolayer-deep depressions on the (100) surface of silicon.

Availability: The facility is operational now. We seek industrial, university, or government partners interested in developing advanced materials whose performance depends on nanometer-scale interfacial structure.

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